

Geometric momentum in the Monge parametrization of two dimensional sphere

D. M. Xun, and Q. H. Liu^{1,*}

¹*School for Theoretical Physics, and Department of Applied Physics, Hunan University, Changsha, 410082, China*
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A two dimensional surface can be considered as three dimensional shell whose thickness is negligible in comparison with the dimension of the whole system. The quantum mechanics on surface can be first formulated in the bulk and the limit of vanishing thickness is then taken. The gradient operator and the Laplace operator originally defined in bulk converges to the geometric ones on the surface, and the so-called geometric momentum and geometric potential are obtained. On the surface of two dimensional sphere the geometric momentum in the Monge parametrization is explicitly explored. Dirac's theory on second-class constrained motion is resorted to for accounting for the commutator $[x_i, p_j] = i\hbar(\delta_{ij} - x_i x_j / r^2)$ rather than $[x_i, p_j] = i\hbar\delta_{ij}$ that does not hold true any more. This geometric momentum is geometric invariant under parameters transformation, and self-adjoint.

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I. INTRODUCTION

It has been a long standing problem how to properly define quantum mechanics on a surface in three dimensional Euclidean space. On one hand, Dirac stressed that in his *Principles* on the canonical quantization assumption that "is found in practice successful only when applied with the dynamic coordinates and momenta referring to a Cartesian system of axes and not to more general curvilinear coordinates." [1] On the other hand, there is in textbooks a routine recipe proposed by DeWitt by hypothesizing the quantum kinetic energy operator to be proportional to Laplace-Beltrami operator Δ_{LB} on the surface, [2]

$$T = -\frac{\hbar^2}{2m}\Delta_{LB}. \quad (1)$$

Is there a way to start from Dirac to reach DeWitt? Certainly, Dirac put forward a theory for systems of second-class constraints [3] which really encompasses the DeWitt's hypothesis as a special case, [4] but contains much more than what was expected.

When we use the tensor covariant and contravariant components and the Einstein summation convention, the so-called standard parametrization $\mathbf{r}(q^1, q^2)$ of the 2D surface is given by,

$$\mathbf{r}(q^1, q^2) = (x(q^1, q^2), y(q^1, q^2), z(q^1, q^2)). \quad (2)$$

In differential geometry, (q^1, q^2) is generally denoted by q^μ and q^ν with lowercase greek letters μ, ν taking values 1, 2, and $\mathbf{r}^\mu = g^{\mu\nu}\mathbf{r}_\nu = g^{\mu\nu}\partial_\nu\mathbf{r} = g^{\mu\nu}\partial\mathbf{r}/q^\nu$ with $g_{\mu\nu} = \partial_\mu\mathbf{r} \cdot \partial_\nu\mathbf{r}$ being the metric tensor. At this point $\mathbf{r}, \mathbf{n} = (n_x, n_y, n_z)$ is the normal and $M\mathbf{n}$ symbolizes the mean curvature vector field, a geometric invariant. [5] In physics, this two dimensional (2D) surface can more realistically be considered as a 3D shell whose thickness is negligible in comparison with the dimension of the whole system. Then, there are two ways to performing the calculus on the surface: Explicitly, when the 2D curved surface is conceived as a limiting case of a curved shell of equal thickness d , where the limit $d \rightarrow 0$ is then taken, great discrepancies present as firstly taking limit $d \rightarrow 0$ then defining the derivatives on the surface, and as firstly defining derivatives in bulk then letting $d \rightarrow 0$. The second order is named as the *confining procedure* for studying motion on 2D surface embedded in 3D. [6–9] This kind of exploration was initialized in 1971, [6] fundamentally finished in 1981, [7] and with correct inclusion of electromagnetic field in 2008 [8] etc. Remarkably, as the *confining procedure* is applied to the momentum operator $\mathbf{p} = -i\hbar\nabla$, we find that the resultant momentum on the surface is with M denoting the mean curvature, [10, 11]

$$\mathbf{p} = -i\hbar(\mathbf{r}^\mu\partial_\mu + M\mathbf{n}), \quad (3)$$

*Electronic address: quanhuiliu@gmail.com

which was originally discovered in 2007 [5] by an entirely independent development on the quantization of the momentum on 2D surface embedded in 3D flat space. This momentum corresponds to the so-called standard parametrization $\mathbf{r}(q^1, q^2)$ of the 2D surface (2) in mathematics therefore should be preferable over other forms of momentum such as the generalized momenta (p_{q^1}, p_{q^2}) canonically conjugated to parameters (q^1, q^2) . Paralleling to the confining procedure-induced *geometric potential* $V_{gp} \equiv -\hbar^2/2m(M^2 - K)$ with K being the gaussian curvature, [12, 13] we call (3) *geometric momentum*. [11] This scheme of building up quantum mechanics on the surface echoes the historic comments of Dirac on the canonical quantization in his *Principles*. [1]

In 2010, with help of the femtosecond laser writing technology, the optical analogue of the quantum *geometric potential* is experimentally realized and its experimental effects on optical wave packets constrained on curved surfaces are demonstrated. [12] In 2012, the *geometric potential* effects on the electronic properties of materials such as Tomonaga-Luttinger liquids are directly confirmed with an observation of the *in situ* high-resolution ultraviolet photoemission spectra of a one-dimensional metallic C_{60} polymer with an uneven periodic peanut-shaped structure. [14] These two experimental verifications may have influences on further developments of physics and mathematics for the 2D curved surfaces, for the *geometric momentum* and the *geometric potential* are, upon two constant factors, the gradient and Laplacian operator, respectively, as pointed out in Refs. [10, 11].

The principal purpose of this study is to explicitly show that, with use of the Monge parametrization of the 2D surface, the geometric momentum is compatible with Dirac's theory for systems of second-class constraints all around.

II. GEOMETRIC MOMENTUM WITH CARTESIAN VARIABLES (x, y)

By Monge parametrization, we mean that a 2D surface given by the form $z = f(x, y)$ where (x, y, z) are Cartesian variables. For a sphere of radius r in R^3 , we have the so-called standard form,

$$\mathbf{r}(x, y) = (x, y, \sqrt{r^2 - x^2 - y^2}). \quad (4)$$

The covariant derivatives \mathbf{r}_μ and contravariant derivatives \mathbf{r}^μ can be easily computed and the results are respectively,

$$\begin{pmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{pmatrix} = \begin{pmatrix} 1, & 0, & -x/\sqrt{r^2 - x^2 - y^2} \\ 0, & 1, & -y/\sqrt{r^2 - x^2 - y^2} \end{pmatrix}, \quad (5)$$

$$\begin{pmatrix} \mathbf{r}^x \\ \mathbf{r}^y \end{pmatrix} \equiv \begin{pmatrix} g^{x\mu} \mathbf{r}_\mu \\ g^{y\mu} \mathbf{r}_\mu \end{pmatrix} = \frac{1}{r^2} \begin{pmatrix} r^2 - x^2, & -xy, & -x\sqrt{r^2 - x^2 - y^2} \\ -xy, & r^2 - y^2, & -y\sqrt{r^2 - x^2 - y^2} \end{pmatrix}. \quad (6)$$

The normal \mathbf{n} and the mean curvature M are given by respectively,

$$\mathbf{n} = \frac{1}{r}(x, y, \sqrt{r^2 - x^2 - y^2}), \quad M = -\frac{1}{r}. \quad (7)$$

Then, the geometric momentum operators p_i ($i = x, y, z$) are,

$$p_x = -i\hbar \frac{1}{r^2}((r^2 - x^2) \frac{\partial}{\partial x} - xy \frac{\partial}{\partial y} - x), \quad (8)$$

$$p_y = -i\hbar \frac{1}{r^2}(-xy \frac{\partial}{\partial x} + (r^2 - y^2) \frac{\partial}{\partial y} - y), \quad (9)$$

$$p_z = i\hbar \frac{\sqrt{r^2 - x^2 - y^2}}{r^2} (x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} + 1). \quad (10)$$

In flat space, we take commutator $[x_i, p_j] = i\hbar \delta_{ij}$ for granted. But we can easily verify that on the sphere the correct results turn out to be $[x_i, p_j] = i\hbar (\delta_{ij} - x_i x_j / r^2)$ with use of (8)- (10). In next section, we will show that we need the Dirac's theory for systems of second-class constraints which accounts for this fact.

III. DIRAC'S THEORY FOR SYSTEMS OF SECOND-CLASS CONSTRAINTS

On the sphere in the Monge parameterization, the primary Hamiltonian H_p is, [3]

$$H_p = \frac{p_i^2}{2m} + \lambda \left(\sqrt{r^2 - x^2 - y^2} - z \right) + up_\lambda, \quad (11)$$

where λ is the Lagrangian multiplier enforcing the constrained of motion on the surface, and u is also a Lagrangian multiplier guaranteeing that this Hamiltonian is defined on the symplectic manifold, and p_i ($i = x, y, z$) and p_λ are respectively the canonical momenta conjugate to variables x_i and λ . The Poisson bracket is defined by.

$$\{f, H_p\} \equiv \frac{\partial f}{\partial x_i} \frac{\partial H_p}{\partial p_i} + \frac{\partial f}{\partial \lambda} \frac{\partial H_p}{\partial p_\lambda} - \left(\frac{\partial f}{\partial p_i} \frac{\partial H_p}{\partial x_i} + \frac{\partial f}{\partial p_\lambda} \frac{\partial H_p}{\partial \lambda} \right). \quad (12)$$

The equations of motion for (x, y, z, λ) are given by,

$$p_i = m\dot{x}, \quad p_\lambda = 0. \quad (13)$$

The primary constraint is then,

$$\varphi_1 = p_\lambda \approx 0, \quad (14)$$

hereafter symbol " \approx " implies a weak equality. After all calculations are finished, weak equality takes back the strong one. The secondary constraints (not confusing with second-class constraints) are then determined by,

$$\{\varphi_i, H_p\} \approx 0. \quad (15)$$

And the complete secondary constraints are,

$$\varphi_2 = \sqrt{r^2 - x^2 - y^2} - z \approx 0, \quad (16)$$

$$\varphi_3 = \frac{xp_x + yp_y}{m\sqrt{r^2 - x^2 - y^2}} + \frac{p_z}{m} \approx 0, \quad (17)$$

$$\varphi_4 = \frac{(r^2 - x^2 - y^2)(p_x^2 + p_y^2 + p_z^2) - r^2\sqrt{r^2 - x^2 - y^2}m\lambda}{m^2(r^2 - x^2 - y^2)^{3/2}} \approx 0, \quad (18)$$

$$\varphi_5 = \frac{p_z(p_x^2 + p_y^2 + p_z^2) + r^2m^2u}{m^3(r^2 - x^2 - y^2)} \approx 0. \quad (19)$$

Eqs. (18) and (19) determine the Lagrangian multipliers λ and u respectively. With introduction of the Dirac bracket instead of the Poisson one for the canonical variables A and B , [3]

$$\{A, B\}_D = \{A, B\} - \{A, \varphi_\alpha\} C_{\alpha\beta}^{-1} \{\varphi_\beta, B\}, \quad (20)$$

which the matrix elements $C_{\alpha\beta}$ ($\alpha, \beta = 1, 2, 3, 4$) is defined by,

$$C_{\alpha\beta} = \{\varphi_\alpha, \varphi_\beta\}, \quad (21)$$

the positions x_i and the momenta p_i satisfy following Dirac bracket, [4, 15–23]

$$\begin{aligned} \{x_i, x_j\}_D &= 0, \quad \{x_i, p_j\}_D = \delta_{ij} - \frac{x_i x_j}{r^2}, \\ \{p_i, p_j\}_D &= -\frac{1}{r^2}(x_i p_j - x_j p_i), \end{aligned} \quad (22)$$

and other Dirac brackets between x_i and p_j vanish. The equation of motion is in general

$$\dot{f} = \{f, H_p\}_D, \quad (23)$$

from which we have for x_i and p_i respectively,

$$\dot{x}_i = \{x_i, H_p\}_D = \frac{p_i}{m}, \quad (24)$$

$$\dot{p}_i = \{p_i, H_p\}_D = -\frac{x_i p_i^2}{mr^2}. \quad (25)$$

Note that in these calculations (23), (24) and (25) where the constraints are of second-class, we need to deal with H instead of H_p for we have,

$$\dot{f} = \{f, H_p\}_D = \{f, H\}_D. \quad (26)$$

In quantum mechanics, the Hamiltonian is, [6, 7]

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\partial_\mu\sqrt{g}g^{\mu\nu}\partial_\nu + V_{gp} \\ &= -\frac{\hbar^2}{2m}\left(\frac{r^2-x^2}{r^2}\frac{\partial^2}{\partial x^2} - \frac{2xy}{r^2}\frac{\partial}{\partial x}\frac{\partial}{\partial y} - \frac{2x}{r^2}\frac{\partial}{\partial x} - \frac{2y}{r^2}\frac{\partial}{\partial y} + \frac{r^2-y^2}{r^2}\frac{\partial^2}{\partial y^2}\right) + V_{gp} \end{aligned} \quad (27)$$

where the factor $g \equiv \det(g_{\mu\nu})$ is the determinant of the matrix $g_{\mu\nu}$, and the geometric potential $V_{gp} = 0$ for $M^2 - K = 0$ on sphere. The quantum commutator $[A, B]$ of two variables A and B is attainable by direct correspondence of the Dirac bracket as $[A, B]/i\hbar \rightarrow \{A, B\}_D$, and the fundamental commutators are:

$$[x_i, x_j] = 0, \quad (28)$$

$$[x_i, p_j] = i\hbar\left(\delta_{ij} - \frac{x_i x_j}{r^2}\right), \quad (29)$$

$$[p_i, p_j] = -\frac{i\hbar}{r^2}(x_i p_j - x_j p_i), \quad (30)$$

There is no operator ordering problem in the right-hand side of Eq. (30) because the commutator must satisfy the Jacobian identity. It is easily to verify that operators p_i (8)-(10) satisfy relations (28)-(30). The second category of the fundamental commutators is given by quantization of (24) and (25)

$$[x_i, H] = i\hbar\frac{p_i}{m}, \quad (31)$$

$$[p_i, H] = -i\hbar\frac{x_i H + H x_i}{mr^2}. \quad (32)$$

Strikingly, the geometric momentum (8)-(10) satisfies all commutators (29)-(32) above, not only (29)-(30). As pointed out in Ref. [10], the usual canonical momentum p_θ violates the fundamental commutator (32).

IV. THE SELF-ADJOINTNESS OF THE GEOMETRIC MOMENTUM

By a self-adjoint operator, we mean that all eigenvalues of it are real, and eigenfunctions corresponding to distinct eigenvalues are mutually orthogonal and they form a complete set. But direct demonstration of the self-adjointness of the geometric momentum (8)-(10) is relatively difficult. With variable transform $(x, y, z) \rightarrow (r, \theta, \varphi)$ with $\theta \in (0, \pi), \varphi \in (0, 2\pi)$ as,

$$\mathbf{r}(\theta, \varphi) = (r \sin \theta \cos \varphi, r \sin \theta \sin \varphi, r \cos \theta) \quad (33)$$

being made, the task becomes easy. The geometric momentum operators in terms of (θ, φ) take following forms, [5, 24, 25]

$$p_x = -\frac{i\hbar}{r}\left(\cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} - \sin \theta \cos \varphi\right), \quad (34)$$

$$p_y = -\frac{i\hbar}{r}\left(\cos \theta \sin \varphi \frac{\partial}{\partial \theta} - \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} - \sin \theta \sin \varphi\right), \quad (35)$$

$$p_z = -\frac{i\hbar}{r}\left(-\sin \theta \frac{\partial}{\partial \theta} - \cos \theta\right). \quad (36)$$

Their complete solutions to eigenvalue equations $p_j(\theta, \varphi)\psi_{p_j}(\theta, \varphi) = p_j\psi_{p_j}(\theta, \varphi)$ can be easily determined. To note that the eigenvalues p_j on the right hand side of these equations differ from the operators $p_j(\theta, \varphi)$ on the left hand side. Explicitly, the solutions are, [26]

$$\psi_{p_x}(\theta, \varphi) = f_x \left(\frac{1 + \sin \theta \cos \varphi}{1 - \sin \theta \cos \varphi}\right)^{irp_x/2\hbar} \frac{\sqrt{\cos \theta \sin \theta \sin \varphi}}{1 - \sin^2 \theta \cos^2 \varphi}, \quad (37)$$

$$\psi_{p_y}(\theta, \varphi) = f_y \left(\frac{1 + \sin \theta \sin \varphi}{1 - \sin \theta \sin \varphi}\right)^{irp_y/2\hbar} \frac{\sqrt{\cos \theta \sin \theta \cos \varphi}}{1 - \sin^2 \theta \sin^2 \varphi}, \quad (38)$$

$$\psi_{p_z}(\theta, \varphi) = C_z \left(\cot \frac{\theta}{2}\right)^{irp_z/\hbar} \frac{1}{\sin \theta}, \quad (39)$$

where f_x and f_y are two arbitrary functions of the same variable $\tan \theta \sin \varphi$. In terms of variables (x, y, z) , we have from (37)-(39),

$$\psi_{p_x}(x, y) = f_x \left(\frac{r+x}{r-x} \right)^{irp_x/2\hbar} \frac{r}{r^2-x^2} \sqrt{y\sqrt{r^2-x^2-y^2}}, \quad (40)$$

$$\psi_{p_y}(x, y) = f_y \left(\frac{r+y}{r-y} \right)^{irp_y/2\hbar} \frac{r}{r^2-y^2} \sqrt{x\sqrt{r^2-x^2-y^2}}, \quad (41)$$

$$\psi_{p_z}(x, y) = C_z \left(\frac{r + \sqrt{r^2-x^2-y^2}}{\sqrt{x^2+y^2}} \right)^{irp_z/\hbar} \frac{r}{\sqrt{x^2+y^2}}, \quad (42)$$

where f_x and f_y are two arbitrary functions of variable $y/\sqrt{r^2-x^2-y^2}$. One can then verify that $p_j(x, y)\psi_{p_j}(x, y) = p_j\psi_{p_j}(x, y)$ are satisfied with geometric momentum of form (8)-(10).

V. REMARKS AND SUMMARY

Two dimensional surface can be considered as three dimensional shell whose thickness is negligible in comparison with the dimension of the whole system. We can study the quantum mechanics on surface by first formulating it in the bulk, and then taking the limit of vanishing thickness, the gradient operator and the Laplace operator originally defined in flat space converges to the geometric ones. The presence of the geometric momentum and geometric potential well reflects the Dirac's penetrating insight into the canonical quantization.

On the two dimensional sphere embedded in three dimensional flat space, the geometric momentum in the Monge parameterization is extensively explored in this paper. The apparent commutator $[x_i, p_j] = i\hbar\delta_{ij}$ does not hold true any more, and we must resort to the Dirac's theory on second-class constrained motion. The correct results turn out to be $[x_i, p_j] = i\hbar(\delta_{ij} - x_i x_j / r^2)$. This geometric momentum is geometric invariant under parameters transformation, and self-adjoint.

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